



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 04:03 am BST

PDB ID : 6QYQ
Title : Crystal structure of human thymidylate synthase (hTS) variant R175C
Authors : Pozzi, C.; Mangani, M.
Deposited on : 2019-03-09
Resolution : 2.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

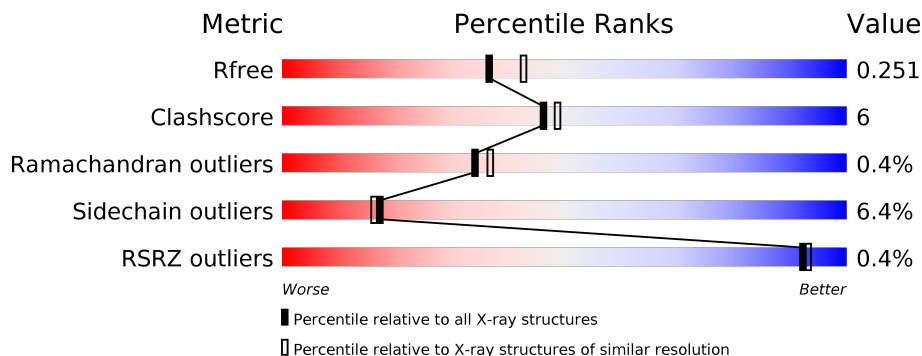
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	325	 73% 14% • 12%
2	C	325	 74% 12% • 12%
3	B	325	 73% 15% • 11%
4	D	325	 74% 13% • 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	SCH	A	180	-	-	X	-
3	SCH	B	180	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 9722 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	286	2275	1459	386	415	15	0	0	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP P04818
A	-10	ARG	-	expression tag	UNP P04818
A	-9	GLY	-	expression tag	UNP P04818
A	-8	SER	-	expression tag	UNP P04818
A	-7	HIS	-	expression tag	UNP P04818
A	-6	HIS	-	expression tag	UNP P04818
A	-5	HIS	-	expression tag	UNP P04818
A	-4	HIS	-	expression tag	UNP P04818
A	-3	HIS	-	expression tag	UNP P04818
A	-2	HIS	-	expression tag	UNP P04818
A	-1	GLY	-	expression tag	UNP P04818
A	0	SER	-	expression tag	UNP P04818
A	175	CYS	ARG	engineered mutation	UNP P04818

- Molecule 2 is a protein called Thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	285	2272	1455	386	416	15	0	0	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-11	MET	-	initiating methionine	UNP P04818
C	-10	ARG	-	expression tag	UNP P04818
C	-9	GLY	-	expression tag	UNP P04818

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	SER	-	expression tag	UNP P04818
C	-7	HIS	-	expression tag	UNP P04818
C	-6	HIS	-	expression tag	UNP P04818
C	-5	HIS	-	expression tag	UNP P04818
C	-4	HIS	-	expression tag	UNP P04818
C	-3	HIS	-	expression tag	UNP P04818
C	-2	HIS	-	expression tag	UNP P04818
C	-1	GLY	-	expression tag	UNP P04818
C	0	SER	-	expression tag	UNP P04818
C	175	CYS	ARG	engineered mutation	UNP P04818

- Molecule 3 is a protein called Thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	B	289	2296	1471	393	415	17	0	0	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	MET	-	initiating methionine	UNP P04818
B	-10	ARG	-	expression tag	UNP P04818
B	-9	GLY	-	expression tag	UNP P04818
B	-8	SER	-	expression tag	UNP P04818
B	-7	HIS	-	expression tag	UNP P04818
B	-6	HIS	-	expression tag	UNP P04818
B	-5	HIS	-	expression tag	UNP P04818
B	-4	HIS	-	expression tag	UNP P04818
B	-3	HIS	-	expression tag	UNP P04818
B	-2	HIS	-	expression tag	UNP P04818
B	-1	GLY	-	expression tag	UNP P04818
B	0	SER	-	expression tag	UNP P04818
B	175	CYS	ARG	engineered mutation	UNP P04818

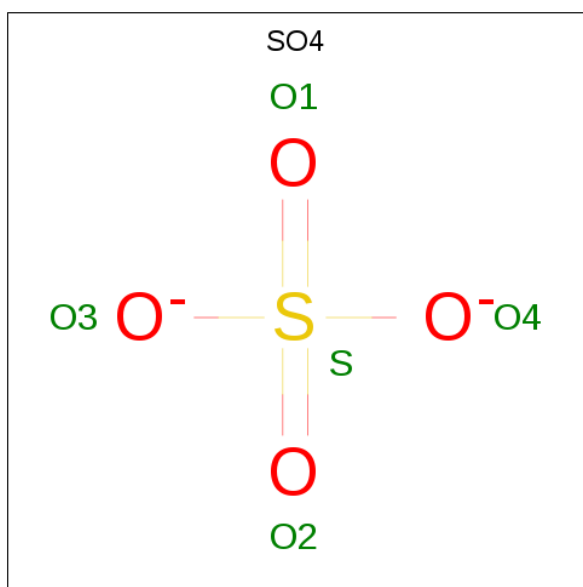
- Molecule 4 is a protein called Thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	290	2303	1476	391	420	16	0	0	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-11	MET	-	initiating methionine	UNP P04818
D	-10	ARG	-	expression tag	UNP P04818
D	-9	GLY	-	expression tag	UNP P04818
D	-8	SER	-	expression tag	UNP P04818
D	-7	HIS	-	expression tag	UNP P04818
D	-6	HIS	-	expression tag	UNP P04818
D	-5	HIS	-	expression tag	UNP P04818
D	-4	HIS	-	expression tag	UNP P04818
D	-3	HIS	-	expression tag	UNP P04818
D	-2	HIS	-	expression tag	UNP P04818
D	-1	GLY	-	expression tag	UNP P04818
D	0	SER	-	expression tag	UNP P04818
D	175	CYS	ARG	engineered mutation	UNP P04818

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0

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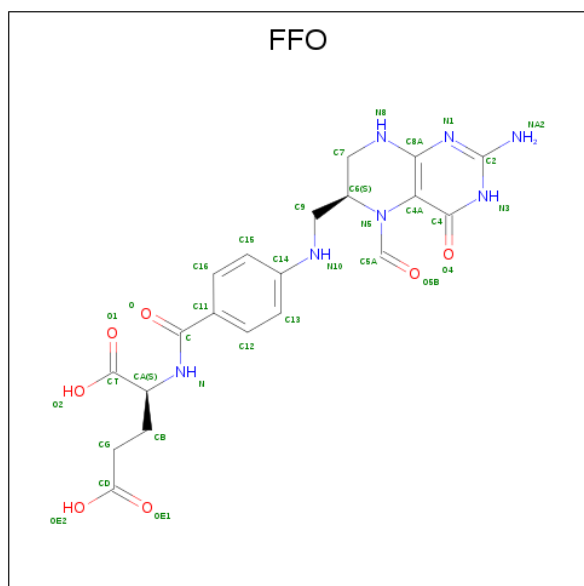
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cl	0	0
			1	1		
6	A	1	Total	Cl	0	0
			1	1		
6	C	2	Total	Cl	0	0
			2	2		

- Molecule 7 is N-[4-({[(6S)-2-amino-5-formyl-4-oxo-3,4,5,6,7,8-hexahydropteridin-6-yl]methyl}amino)benzoyl]-L-glutamic acid (three-letter code: FFO) (formula: C₂₀H₂₃N₇O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			34	20	7	7		
7	D	1	Total	C	N	O	0	0
			34	20	7	7		

- Molecule 8 is water.

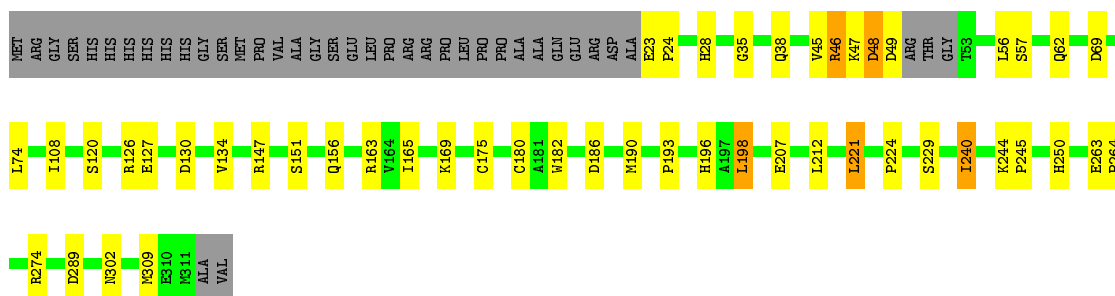
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	152	Total 152	O 152	0	0
8	C	120	Total 120	O 120	0	0
8	B	102	Total 102	O 102	0	0
8	D	100	Total 100	O 100	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

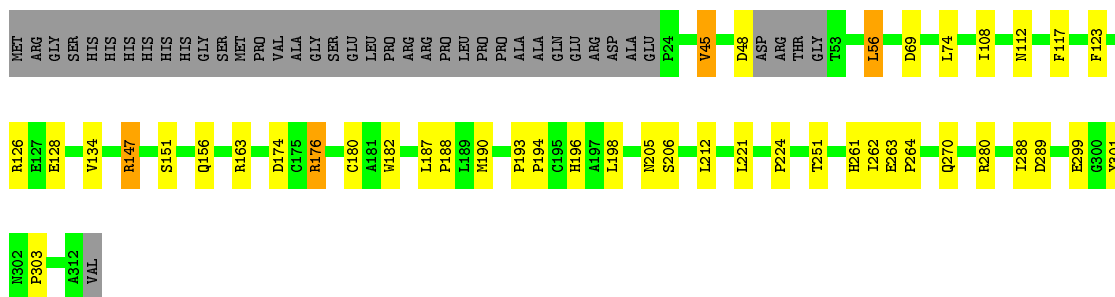
- Molecule 1: Thymidylate synthase

Chain A: 




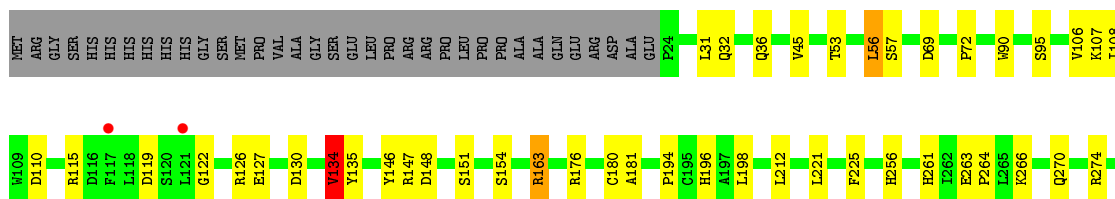
- Molecule 2: Thymidylate synthase

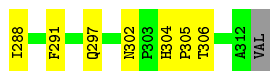
Chain C: 



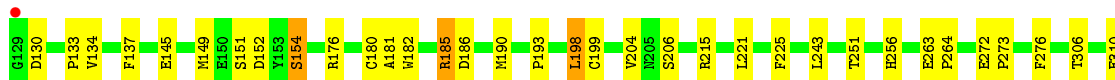
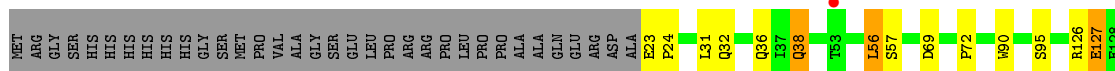
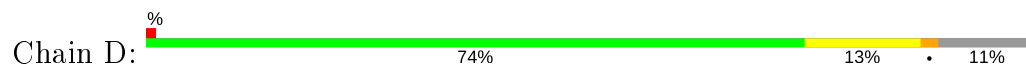
- Molecule 3: Thymidylate synthase

Chain B: 





- Molecule 4: Thymidylate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.49Å 96.52Å 139.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.70 – 2.25 36.67 – 2.25	Depositor EDS
% Data completeness (in resolution range)	92.5 (36.70-2.25) 92.5 (36.67-2.25)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.42 (at 2.24Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.183 , 0.251 0.183 , 0.251	Depositor DCC
R_{free} test set	2917 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	37.5	Xtrriage
Anisotropy	0.204	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 32.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.449 for k,h,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9722	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SCH, CL, CME, FFO, CSX, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.58	0/2307	0.93	0/3125
2	C	0.58	0/2294	0.95	0/3106
3	B	0.49	0/2320	0.89	1/3140 (0.0%)
4	D	0.51	0/2336	0.90	0/3165
All	All	0.54	0/9257	0.92	1/12536 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	163	ARG	CG-CD-NE	-5.12	101.05	111.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2275	0	2191	33	0
2	C	2272	0	2185	34	0
3	B	2296	0	2210	34	0
4	D	2303	0	2214	31	0
5	A	15	0	0	0	0
5	B	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	5	0	0	1	0
5	D	5	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	2	0	0	0	0
7	B	34	0	21	0	0
7	D	34	0	21	0	0
8	A	152	0	0	2	0
8	B	102	0	0	1	0
8	C	120	0	0	3	0
8	D	100	0	0	2	0
All	All	9722	0	8842	113	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (113) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:180:CME:HZ2	4:D:182:TRP:HB3	1.51	0.93
3:B:122:GLY:HA2	8:B:578:HOH:O	1.73	0.87
4:D:38:GLN:HG3	8:D:515:HOH:O	1.74	0.86
1:A:74:LEU:HD12	1:A:224:PRO:HB3	1.64	0.79
2:C:45:VAL:CG2	4:D:204:VAL:HG21	2.15	0.76
5:C:401:SO4:O4	4:D:176:ARG:HD2	1.88	0.73
1:A:182:TRP:HB3	3:B:180:SCH:HE2	1.70	0.71
4:D:263:GLU:HB2	4:D:264:PRO:HD3	1.71	0.71
2:C:45:VAL:HG21	4:D:204:VAL:HG21	1.72	0.71
2:C:176:ARG:HD3	4:D:193:PRO:HG3	1.76	0.68
4:D:23:GLU:CD	4:D:24:PRO:HD3	2.15	0.66
3:B:126:ARG:HG2	3:B:130:ASP:HB3	1.78	0.65
2:C:45:VAL:HG21	4:D:204:VAL:CG2	2.28	0.64
1:A:263:GLU:HB2	1:A:264:PRO:HD3	1.79	0.64
2:C:301:TYR:CE2	2:C:303:PRO:HG3	2.33	0.64
1:A:182:TRP:HB3	3:B:180:SCH:CE	2.28	0.63
2:C:182:TRP:HH2	4:D:176:ARG:HG2	1.63	0.63
4:D:126:ARG:HG2	4:D:130:ASP:HB3	1.81	0.61
1:A:126:ARG:HG2	1:A:130:ASP:HB3	1.81	0.61
2:C:147:ARG:NH2	2:C:156:GLN:OE1	2.33	0.61
1:A:221:LEU:C	1:A:221:LEU:HD13	2.21	0.60
2:C:147:ARG:HH21	2:C:156:GLN:HE22	1.48	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:TRP:HH2	3:B:176:ARG:HG2	1.68	0.58
2:C:180:CME:OH	4:D:180:CYS:SG	2.60	0.57
1:A:180:SCH:HE2	3:B:180:SCH:HE1	1.85	0.57
1:A:198:LEU:C	1:A:198:LEU:HD12	2.25	0.57
2:C:205:ASN:O	2:C:206:SER:HB2	2.04	0.56
1:A:147:ARG:NH2	1:A:156:GLN:OE1	2.39	0.56
2:C:270:GLN:HG2	8:C:611:HOH:O	2.05	0.56
4:D:181:ALA:HB2	4:D:199:CME:HZ2	1.88	0.56
3:B:288:ILE:HD12	3:B:291:PHE:CE2	2.41	0.55
2:C:156:GLN:NE2	8:C:501:HOH:O	2.41	0.54
1:A:180:SCH:HE1	3:B:180:SCH:CE	2.38	0.54
2:C:263:GLU:HB2	2:C:264:PRO:HD3	1.89	0.54
3:B:115:ARG:HD3	3:B:119:ASP:CG	2.28	0.53
3:B:56:LEU:O	3:B:256:HIS:HA	2.08	0.53
2:C:74:LEU:HD12	2:C:224:PRO:HB3	1.91	0.53
2:C:198:LEU:HD12	2:C:198:LEU:C	2.28	0.53
1:A:48:ASP:OD1	1:A:48:ASP:N	2.42	0.53
2:C:180:CME:HH	4:D:180:CYS:HG	1.53	0.53
4:D:198:LEU:HD12	4:D:198:LEU:C	2.29	0.53
1:A:182:TRP:CD1	3:B:180:SCH:HE2	2.44	0.53
3:B:196:HIS:HB3	3:B:212:LEU:HD11	1.91	0.52
2:C:280:ARG:HG2	2:C:280:ARG:HH11	1.75	0.52
1:A:35:GLY:HA2	1:A:38:GLN:HG2	1.92	0.51
4:D:23:GLU:N	4:D:24:PRO:CD	2.73	0.51
3:B:32:GLN:O	3:B:36:GLN:HG3	2.11	0.51
4:D:145:GLU:OE1	4:D:185:ARG:NH1	2.44	0.51
1:A:180:SCH:CE	3:B:180:SCH:HE1	2.42	0.50
2:C:196:HIS:HB3	2:C:212:LEU:HD11	1.94	0.50
2:C:123:PHE:HB3	2:C:126:ARG:HG3	1.93	0.50
2:C:147:ARG:HG3	2:C:151:SER:OG	2.12	0.49
3:B:263:GLU:HB2	3:B:264:PRO:HD3	1.93	0.49
1:A:180:SCH:CE	3:B:180:SCH:CE	2.90	0.49
3:B:261:HIS:C	3:B:264:PRO:HD2	2.33	0.49
1:A:207:GLU:HA	1:A:244:LYS:O	2.13	0.48
2:C:112:ASN:HA	2:C:117:PHE:CD2	2.48	0.48
1:A:28:HIS:NE2	1:A:274:ARG:O	2.45	0.48
4:D:206:SER:HA	4:D:243:LEU:HD22	1.95	0.48
4:D:32:GLN:O	4:D:36:GLN:HG3	2.13	0.47
3:B:274:ARG:HD3	3:B:302:ASN:O	2.15	0.47
2:C:263:GLU:N	2:C:264:PRO:CD	2.77	0.47
3:B:198:LEU:HD12	3:B:198:LEU:C	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:261:HIS:C	2:C:264:PRO:HD2	2.36	0.47
3:B:304:HIS:HB3	3:B:305:PRO:HD2	1.97	0.46
1:A:263:GLU:N	1:A:264:PRO:CD	2.78	0.46
3:B:146:TYR:CD1	3:B:147:ARG:N	2.84	0.46
2:C:280:ARG:HG2	2:C:280:ARG:NH1	2.31	0.45
1:A:221:LEU:HD22	1:A:221:LEU:O	2.16	0.45
2:C:187:LEU:N	2:C:188:PRO:HD2	2.32	0.45
1:A:23:GLU:HB3	1:A:24:PRO:HD3	2.00	0.44
1:A:196:HIS:HB3	1:A:212:LEU:HD11	2.00	0.44
2:C:174:ASP:OD1	2:C:176:ARG:N	2.47	0.44
2:C:180:CME:HH	4:D:180:CYS:CB	2.29	0.44
2:C:182:TRP:CZ2	2:C:187:LEU:HD11	2.52	0.44
1:A:244:LYS:HB2	1:A:244:LYS:HE3	1.80	0.44
4:D:263:GLU:CB	4:D:264:PRO:HD3	2.44	0.43
2:C:193:PRO:HD3	8:C:564:HOH:O	2.18	0.43
3:B:288:ILE:HD12	3:B:291:PHE:CD2	2.54	0.43
3:B:288:ILE:HD12	3:B:291:PHE:HE2	1.82	0.43
1:A:165:ILE:HG12	1:A:240:ILE:HD11	2.00	0.42
3:B:263:GLU:N	3:B:264:PRO:CD	2.81	0.42
3:B:147:ARG:HB2	3:B:148:ASP:H	1.65	0.42
4:D:152:ASP:OD1	4:D:154:SER:HB2	2.19	0.42
3:B:181:ALA:O	3:B:194:PRO:HG2	2.20	0.42
2:C:56:LEU:HD22	2:C:262:ILE:HD11	2.00	0.42
1:A:274:ARG:HD3	1:A:302:ASN:O	2.19	0.42
1:A:46:ARG:HG3	1:A:47:LYS:N	2.34	0.42
1:A:309:MET:HA	8:A:533:HOH:O	2.19	0.42
4:D:72:PRO:HA	4:D:276:PHE:CD1	2.55	0.42
3:B:261:HIS:O	3:B:264:PRO:HD2	2.19	0.42
2:C:187:LEU:HA	2:C:190:MET:HE3	2.02	0.42
2:C:251:THR:HG21	4:D:251:THR:HG21	2.00	0.42
4:D:272:GLU:HA	4:D:273:PRO:HD3	1.91	0.42
3:B:107:LYS:O	3:B:110:ASP:HB2	2.20	0.42
4:D:56:LEU:O	4:D:256:HIS:HA	2.20	0.42
4:D:127:GLU:OE1	4:D:127:GLU:HA	2.20	0.41
3:B:53:THR:HG22	3:B:53:THR:O	2.19	0.41
4:D:90:TRP:HE1	4:D:95:SER:HG	1.68	0.41
4:D:186:ASP:O	4:D:190:MET:HG2	2.21	0.41
3:B:134:VAL:HB	3:B:135:TYR:H	1.77	0.41
1:A:186:ASP:O	1:A:190:MET:HG3	2.20	0.41
1:A:62:GLN:HA	1:A:250:HIS:O	2.19	0.41
4:D:133:PRO:HB3	4:D:137:PHE:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:LYS:HA	1:A:245:PRO:HD3	1.90	0.41
1:A:175:CYS:HB2	5:B:401:SO4:O3	2.21	0.41
1:A:180:SCH:HE1	3:B:180:SCH:HE3	2.02	0.41
3:B:266:LYS:O	3:B:270:GLN:NE2	2.54	0.41
2:C:193:PRO:HA	2:C:194:PRO:HD3	1.84	0.40
1:A:193:PRO:HD3	8:A:582:HOH:O	2.21	0.40
3:B:90:TRP:HE1	3:B:95:SER:HG	1.67	0.40
4:D:310:GLU:HG3	8:D:584:HOH:O	2.21	0.40
3:B:106:VAL:HG12	3:B:108:ILE:HG12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	279/325 (86%)	267 (96%)	11 (4%)	1 (0%)	34	37
2	C	277/325 (85%)	265 (96%)	11 (4%)	1 (0%)	34	37
3	B	283/325 (87%)	264 (93%)	17 (6%)	2 (1%)	22	21
4	D	285/325 (88%)	272 (95%)	12 (4%)	1 (0%)	34	37
All	All	1124/1300 (86%)	1068 (95%)	51 (4%)	5 (0%)	34	37

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	306	THR
4	D	134	VAL
3	B	134	VAL
2	C	134	VAL
1	A	134	VAL

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	236/278 (85%)	218 (92%)	18 (8%)	13	12
2	C	234/277 (84%)	221 (94%)	13 (6%)	21	21
3	B	233/277 (84%)	219 (94%)	14 (6%)	19	18
4	D	236/278 (85%)	221 (94%)	15 (6%)	17	16
All	All	939/1110 (85%)	879 (94%)	60 (6%)	17	16

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	VAL
1	A	46	ARG
1	A	48	ASP
1	A	49	ASP
1	A	56	LEU
1	A	57	SER
1	A	69	ASP
1	A	108	ILE
1	A	120	SER
1	A	127	GLU
1	A	151	SER
1	A	163	ARG
1	A	169	LYS
1	A	198	LEU
1	A	221	LEU
1	A	229	SER
1	A	240	ILE
1	A	289	ASP
2	C	45	VAL
2	C	48	ASP
2	C	56	LEU
2	C	69	ASP
2	C	108	ILE
2	C	128	GLU

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Mol	Chain	Res	Type
2	C	147	ARG
2	C	163	ARG
2	C	176	ARG
2	C	221	LEU
2	C	288	ILE
2	C	289	ASP
2	C	299	GLU
3	B	31	LEU
3	B	45	VAL
3	B	56	LEU
3	B	57	SER
3	B	69	ASP
3	B	72	PRO
3	B	127	GLU
3	B	134	VAL
3	B	151	SER
3	B	154	SER
3	B	163	ARG
3	B	221	LEU
3	B	225	PHE
3	B	297	GLN
4	D	31	LEU
4	D	38	GLN
4	D	56	LEU
4	D	57	SER
4	D	69	ASP
4	D	127	GLU
4	D	149	MET
4	D	151	SER
4	D	154	SER
4	D	185	ARG
4	D	198	LEU
4	D	215	ARG
4	D	221	LEU
4	D	225	PHE
4	D	306	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	211	GLN
3	B	270	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

14 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CME	B	199	3	8,9,10	0.62	0	5,9,11	0.79	0
1	CSX	A	195	1	3,6,7	1.14	0	1,6,8	0.26	0
2	CSX	C	195	2	3,6,7	1.16	0	1,6,8	0.55	0
4	CME	D	199	4	8,9,10	0.48	0	5,9,11	0.73	0
2	CME	C	180	2	8,9,10	0.62	0	5,9,11	1.85	3 (60%)
2	CME	C	199	2	8,9,10	0.61	0	5,9,11	1.17	0
1	CME	A	199	1	8,9,10	0.63	0	5,9,11	1.08	0
3	CSX	B	195	3	3,6,7	0.68	0	1,6,8	0.60	0
4	CSX	D	195	4	3,6,7	0.64	0	1,6,8	0.52	0
2	CSX	C	43	2	3,6,7	0.63	0	1,6,8	3.11	1 (100%)
3	SCH	B	43	3	6,7,8	0.47	0	3,7,9	0.58	0
4	SCH	D	43	4	6,7,8	0.44	0	3,7,9	0.77	0
1	SCH	A	180	1	6,7,8	0.52	0	3,7,9	1.68	1 (33%)
3	SCH	B	180	3	6,7,8	0.55	0	3,7,9	0.90	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CME	B	199	3	-	0/5/8/10	-
1	CSX	A	195	1	-	0/1/5/7	-
2	CSX	C	195	2	-	0/1/5/7	-
4	CME	D	199	4	-	1/5/8/10	-
2	CME	C	180	2	-	4/5/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CME	C	199	2	-	0/5/8/10	-
1	CME	A	199	1	-	0/5/8/10	-
3	CSX	B	195	3	-	0/1/5/7	-
4	CSX	D	195	4	-	0/1/5/7	-
2	CSX	C	43	2	-	0/1/5/7	-
3	SCH	B	43	3	-	0/2/6/8	-
4	SCH	D	43	4	-	0/2/6/8	-
1	SCH	A	180	1	-	2/2/6/8	-
3	SCH	B	180	3	-	0/2/6/8	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	43	CSX	CA-CB-SG	-3.11	106.56	113.36
2	C	180	CME	CB-SG-SD	-2.72	96.77	103.82
2	C	180	CME	OH-CZ-CE	2.28	119.83	110.83
1	A	180	SCH	CB-SG-SD	2.09	109.23	103.82
2	C	180	CME	CZ-CE-SD	2.07	120.55	113.37

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	180	CME	CE-SD-SG-CB
1	A	180	SCH	N-CA-CB-SG
4	D	199	CME	SD-CE-CZ-OH
2	C	180	CME	SD-CE-CZ-OH
2	C	180	CME	CZ-CE-SD-SG
1	A	180	SCH	CA-CB-SG-SD
2	C	180	CME	N-CA-CB-SG

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	199	CME	1	0
2	C	180	CME	4	0
1	A	180	SCH	5	0
3	B	180	SCH	8	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	A	402	-	4,4,4	0.37	0	6,6,6	0.11	0
5	SO4	C	401	-	4,4,4	0.43	0	6,6,6	0.11	0
5	SO4	D	401	-	4,4,4	0.29	0	6,6,6	0.16	0
5	SO4	A	401	-	4,4,4	0.43	0	6,6,6	0.12	0
5	SO4	B	401	-	4,4,4	0.37	0	6,6,6	0.19	0
5	SO4	A	403	-	4,4,4	0.36	0	6,6,6	0.11	0
7	FFO	D	402	-	28,36,36	1.00	3 (10%)	28,50,50	1.38	4 (14%)
7	FFO	B	402	-	28,36,36	0.98	3 (10%)	28,50,50	1.39	5 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	FFO	B	402	-	-	5/18/37/37	0/2/3/3
7	FFO	D	402	-	-	5/18/37/37	0/2/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	402	FFO	C4-N3	3.22	1.38	1.33
7	B	402	FFO	C5A-N5	2.51	1.39	1.35
7	B	402	FFO	C4-N3	2.43	1.37	1.33
7	B	402	FFO	C8A-N1	2.17	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	402	FFO	C5A-N5	2.16	1.38	1.35
7	D	402	FFO	C8A-N1	2.01	1.38	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	402	FFO	C4-C4A-C8A	5.01	118.36	114.44
7	B	402	FFO	C4-C4A-C8A	4.60	118.04	114.44
7	D	402	FFO	C2-N1-C8A	2.90	121.05	114.54
7	B	402	FFO	C2-N1-C8A	2.69	120.57	114.54
7	B	402	FFO	C4-N3-C2	2.61	120.08	115.93
7	B	402	FFO	C4A-N5-C6	-2.38	115.10	119.31
7	D	402	FFO	N3-C2-N1	-2.13	122.07	125.42
7	D	402	FFO	C4-N3-C2	2.08	119.24	115.93
7	B	402	FFO	N3-C2-N1	-2.04	122.22	125.42

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	402	FFO	O5B-C5A-N5-C6
7	D	402	FFO	N5-C6-C9-N10
7	B	402	FFO	N5-C6-C9-N10
7	B	402	FFO	CA-CB-CG-CD
7	B	402	FFO	C7-C6-C9-N10
7	D	402	FFO	O5B-C5A-N5-C4A
7	B	402	FFO	N-CA-CB-CG
7	D	402	FFO	C6-C9-N10-C14
7	B	402	FFO	C6-C9-N10-C14
7	D	402	FFO	C15-C14-N10-C9

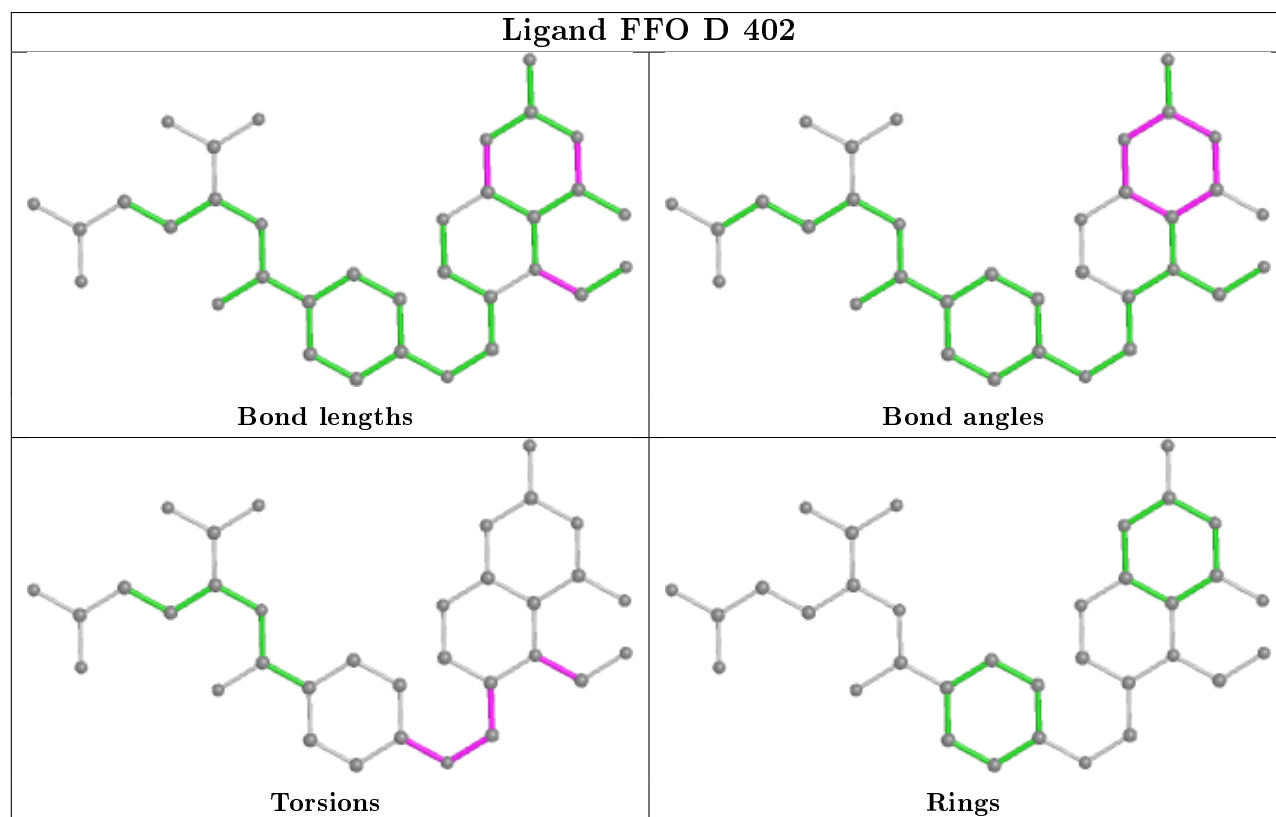
There are no ring outliers.

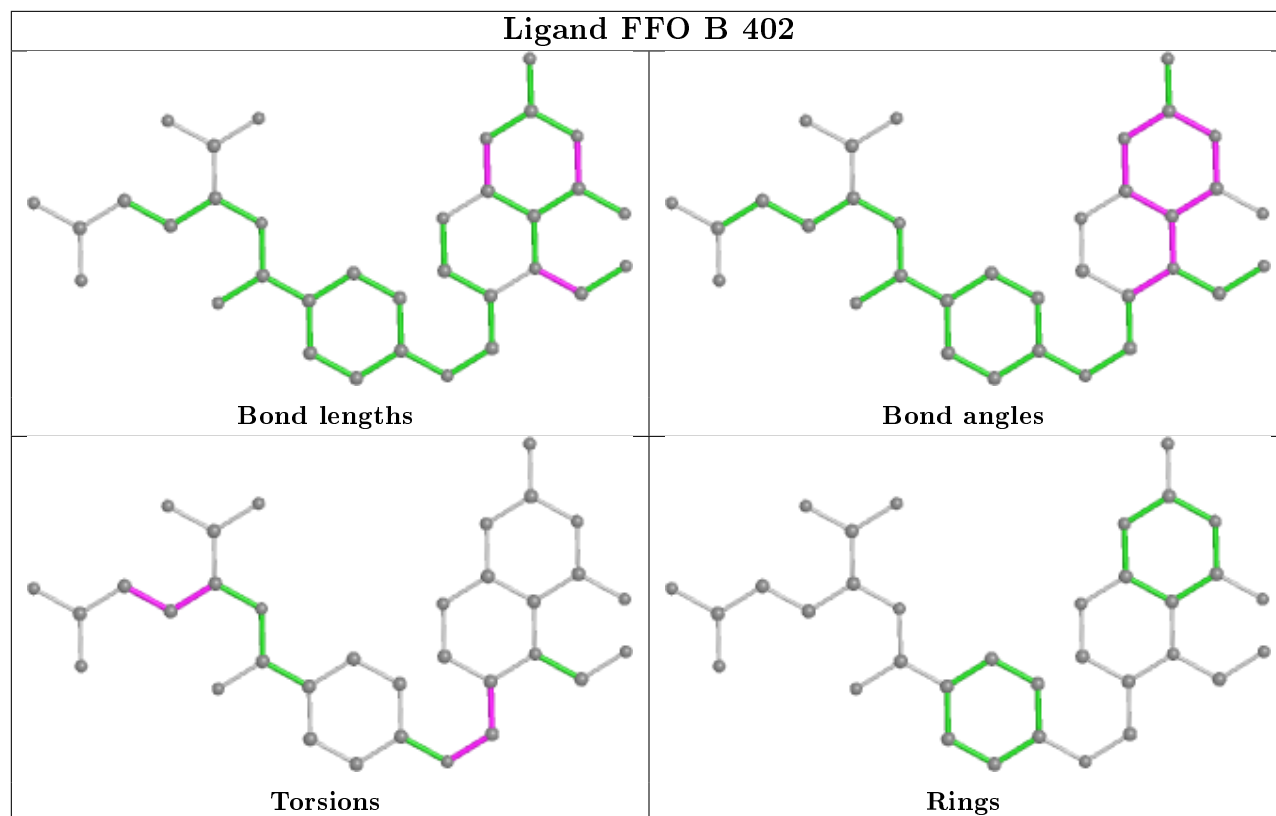
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	401	SO4	1	0
5	B	401	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	283/325 (87%)	-0.62	0 100 100	23, 40, 63, 115	5 (1%)
2	C	281/325 (86%)	-0.61	0 100 100	23, 40, 63, 121	4 (1%)
3	B	285/325 (87%)	-0.44	2 (0%) 87 88	25, 51, 78, 111	4 (1%)
4	D	287/325 (88%)	-0.45	2 (0%) 87 88	29, 49, 85, 105	9 (3%)
All	All	1136/1300 (87%)	-0.53	4 (0%) 92 93	23, 45, 76, 121	22 (1%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	53	THR	2.2
4	D	129	GLY	2.1
3	B	117	PHE	2.1
3	B	121	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CSX	C	43	7/8	0.91	0.12	50,51,65,70	0
1	CME	A	199	10/11	0.92	0.10	29,33,41,42	0
4	CME	D	199	10/11	0.92	0.11	33,38,47,47	0
4	SCH	D	43	8/9	0.92	0.09	44,48,72,73	0
1	SCH	A	180	8/9	0.92	0.12	35,39,74,80	0
3	CME	B	199	10/11	0.93	0.11	32,37,48,49	0
1	CSX	A	195	7/8	0.94	0.09	33,34,35,38	0
2	CME	C	180	10/11	0.94	0.11	35,43,73,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CSX	C	195	7/8	0.94	0.11	31,32,33,35	0
3	SCH	B	43	8/9	0.95	0.08	43,47,55,59	3
4	CSX	D	195	7/8	0.95	0.10	40,44,49,51	0
2	CME	C	199	10/11	0.95	0.09	29,32,39,40	0
3	CSX	B	195	7/8	0.96	0.09	40,43,45,51	0
3	SCH	B	180	8/9	0.96	0.10	38,41,70,71	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

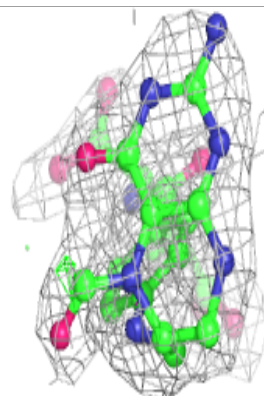
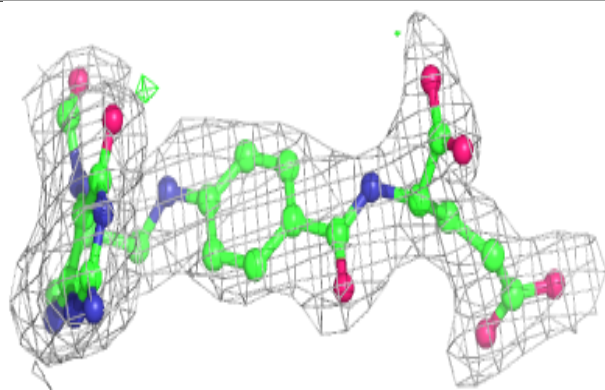
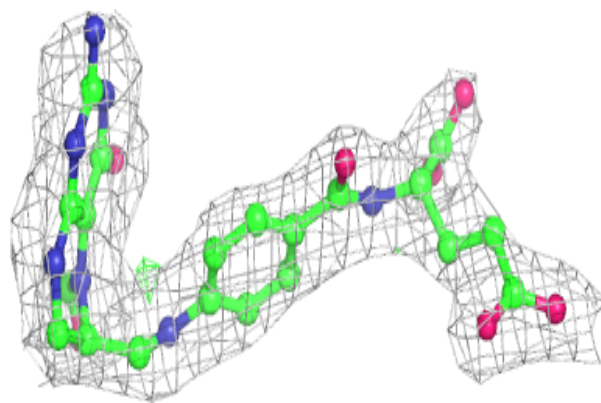
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	CL	A	404	1/1	0.79	0.20	81,81,81,81	0
6	CL	C	402	1/1	0.82	0.13	72,72,72,72	0
7	FFO	D	402	34/34	0.90	0.14	45,59,68,71	0
5	SO4	D	401	5/5	0.91	0.13	58,80,84,86	0
7	FFO	B	402	34/34	0.91	0.15	47,57,65,67	0
5	SO4	A	402	5/5	0.93	0.09	98,98,100,104	0
5	SO4	B	401	5/5	0.94	0.09	48,63,68,72	0
5	SO4	A	403	5/5	0.96	0.07	69,72,75,77	0
6	CL	B	403	1/1	0.96	0.08	73,73,73,73	0
6	CL	C	403	1/1	0.97	0.05	76,76,76,76	0
5	SO4	A	401	5/5	0.98	0.11	54,56,64,64	0
5	SO4	C	401	5/5	0.98	0.10	59,60,63,68	0

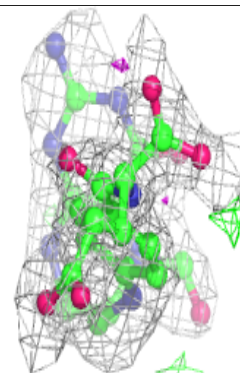
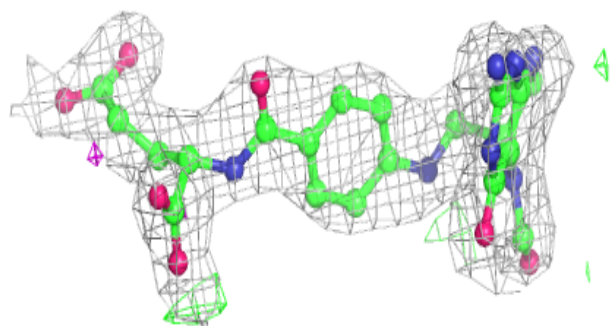
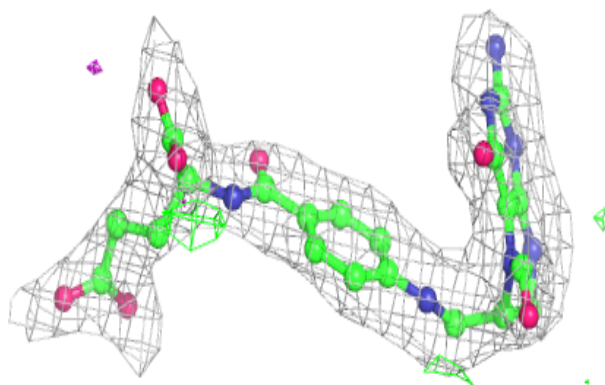
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FFO D 402:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around FFO B 402:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.